LA-UR-11-10053

NJOY & Data Evaluation Status

Presented at the NCSP FY10 Technical Symposium
held at Oak Ridge National Laboratory
March 1 – 2, 2011

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Abstract

We review FY10 Methods and Nuclear Data Evaluation work performed by T-2 for the DOE Nuclear Criticality Safety Program.

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LANL T2 NCSP Summary

- **Program Elements**
  - **Analytical Methods**
    - NJOY Developments
  - **Nuclear Data**
    - Data Evaluations
      - Data Testing
        - Criticality calculations (primarily with ICSBEP benchmarks)
        - Reaction rate ratios (primarily historical LANL measurements)

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Analytical Methods – NJOY Developments

- During FY10 two concurrent versions of NJOY were under development
  - NJOY99.xxx
    - Base Version Released through RSICC and the NEA Databank
      - Update files released via a local (t2.lanl.gov) web site
      - Has worldwide user community

        Local control of updates allows this community to have access to the latest version.

    - Several dozen code patches are typically released each year.
      - NJOY99.304 at the beginning of FY2010
      - NJOY99.336 at the end of FY2010 (plus NJOY99.347 and later have been shared with selected users during the Fall 2010 and Winter 2011 to support ENDF/B-VII.1 development)

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Analytical Methods – NJOY Developments

- NJOY99 enhancements
  - Improved R-M processing in ERRORJ (consistent with RECONR);
  - Refined beta mesh in THERMR for free gas scattering;
  - More robust processing of IRDF (MF10) sections in RECONR, GROUPR & ACER;
  - More efficient processing & error detection in PURR;
  - Improved processing in RECONR, BROADR & ACER for (TENDL-2009) photonuclear and charged particle files;
  - Scattering radius uncertainty processing in ERRORR (via User input or from November, 2009 format revision);
  - MF=40 processing in ERRORR & COVR;
  - Miscellaneous upgrades in RECONR, GROUPR, ACER & ERRORR for JENDL-4 processing;
  - More scratch space in various modules.

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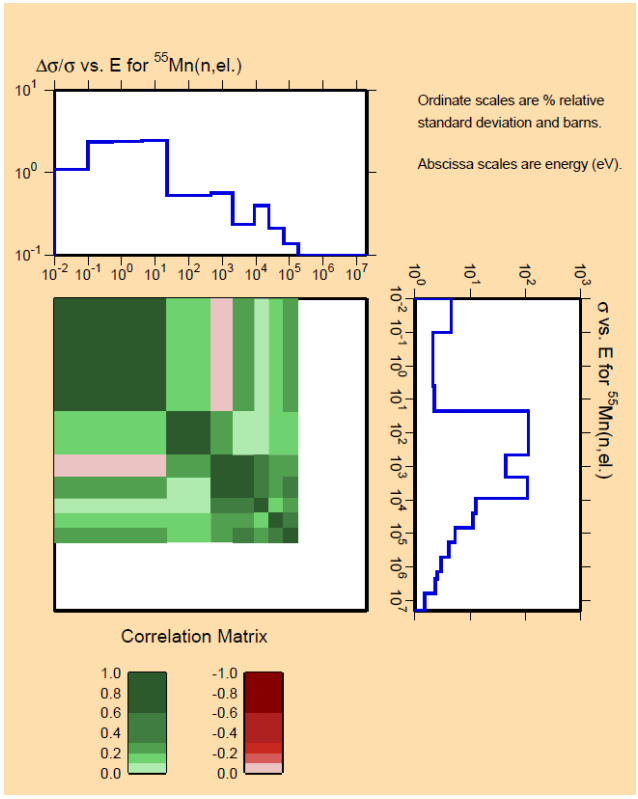
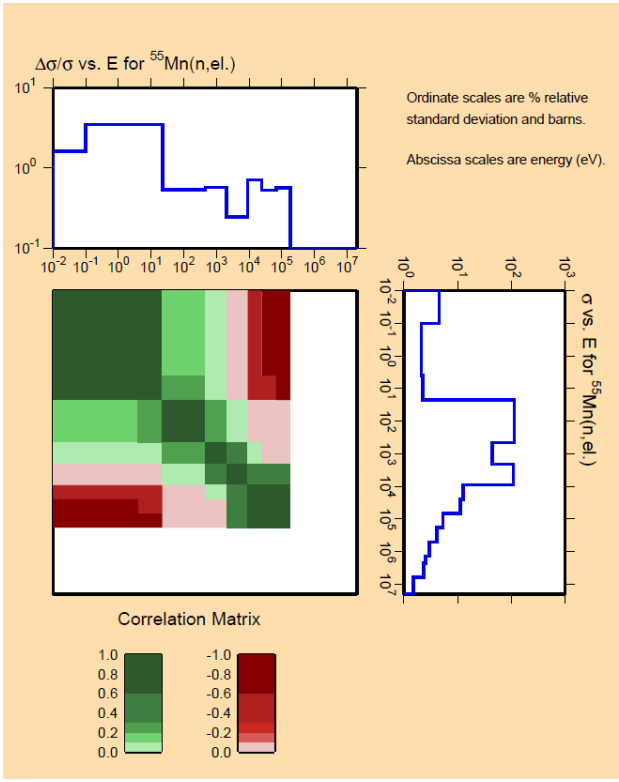
Analytical Methods – NJOY Developments



No scattering radius uncertainty



10% scattering radius uncertainty

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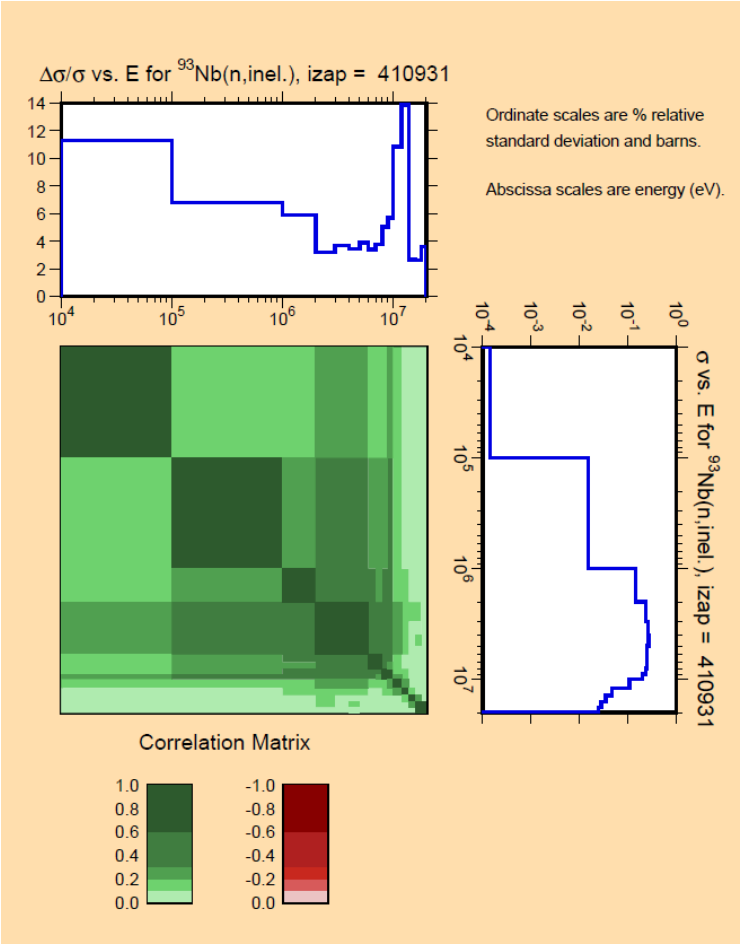
Analytical Methods – NJOY Developments



- ENDF/B-VII.0 ^{93}Nb
  - Includes “10*IZAP+LFS” identifier read from file 40 per the format modification approved at the Fall 2009 CSEWG meeting.
  - Plot format is identical to that produced from file 33 but the presence of the izap label indicates that these are mf40 data.
    - IZAP label identifies the product nuclide and isomer (or ground) state.
  - If IZAP is not given in file 40 the text string “MF40” will appear in the title.

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Analytical Methods – NJOY Developments

- NJOY2010
  - F90/F95 based coding
    - Includes LRF=7 (Limited Reich-Moore resonance format)
      - Appearing in ENDF/A ^{19}F & ^{35}Cl files developed at ORNL and expected to be included in ENDF/B-VII.1
    - "smarter" interpolation for emission spectra (available in NJOY99 but turned off by default)
      - Sqrt(E') rather than histogram at low energy
      - Denser energy grid at high energy
  - Retain all NJOY99 capabilities
  - Internal LA-CC and LA-CP computer code and document numbers have been obtained.
    - Final release to RSICC has been delayed so that last minute upgrades needed for ENDF/B-VII.1 beta processing are incorporated.

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Analytical Methods – NJOY Developments

- "Methods for Processing ENDF/B-VII with NJOY"
- Published in the December 2010 Special Issue on Nuclear Reaction Data of the Nuclear Data Sheets

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www.elsevier.com/locate/nds

Methods for Processing ENDF/B-VII with NJOY

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The NJOY Nuclear Data Processing System is widely used to convert evaluations in the Evaluated Nuclear Data Files (ENDF) format into forms useful for practical applications such as fission and fusion reactor analysis, stockpile stewardship calculations, criticality safety, radiation shielding, nuclear waste management, nuclear medicine procedures, and more. This paper provides a description of the system's capabilities, summary descriptions of the methods used, and information on how to use the code to process the modern evaluated nuclear data files from ENDF/B-VII. It begins with the generation of pointwise libraries, including reaction and resonance reconstruction, Doppler broadening, radiation heating and damage, thermal scattering data, unresolved resonance data, and gas production. It then reviews the production of libraries for the continuous-energy Monte Carlo code MCNP, multigroup neutron, photon, and particle cross sections and matrices, and photon interaction data. The generation of uncertainty information for ENDF data is discussed, including new capabilities for calculating covariances of resonance data, angular distributions, energy distributions, and radioactive nuclide production. NJOY's ability to prepare thermal scattering data evaluations for bound moderators (which was used during the preparation of the ENDF/B-VII library) is described. The strong plotting capabilities of NJOY are summarized. Many examples of black&white and color Postscript plots are included throughout the paper. The capabilities of NJOY to output multigroup data in several different formats to suit various applications is reviewed. Finally, a section is included that summarizes the history of the development of the NJOY system over the last 37 years.

Contents

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Nuclear Data – Evaluations

- ^{4}He, ^{9}Be, ^{16}O – Gerry Hale
- ^{50,51}V – Toshihiko Kawano
- ^{237}Np – Shannon Holloway
- Fission Spectra – Patrick Talou
  - Data Testing – Skip Kahler & Bob MacFarlane

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Nuclear Data – Evaluations – ^{4}He

- Update of 1973 Evaluation.
- New multi-channel R-Matrix Analysis Includes Data from (n + ^{4}He) and (d + t) Systems.
- Includes Covariance Data for Total and Elastic Scattering Cross Sections.

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Nuclear Data – Evaluations – ^{9}Be

- Single-channel fit to the total cross section (including new RPI data) at energies up to 14 MeV.
- Preliminary criticality testing indicates k_{calc} values for Be reflected assemblies have moved back toward ENDF/B-VI levels.
- Full multi-channel R-matrix analysis of reactions in the ^{10}Be system continues.
  - Changes in the elastic scattering angular distributions may affect integral data testing.
  - Covariances for all cross sections will be obtained.

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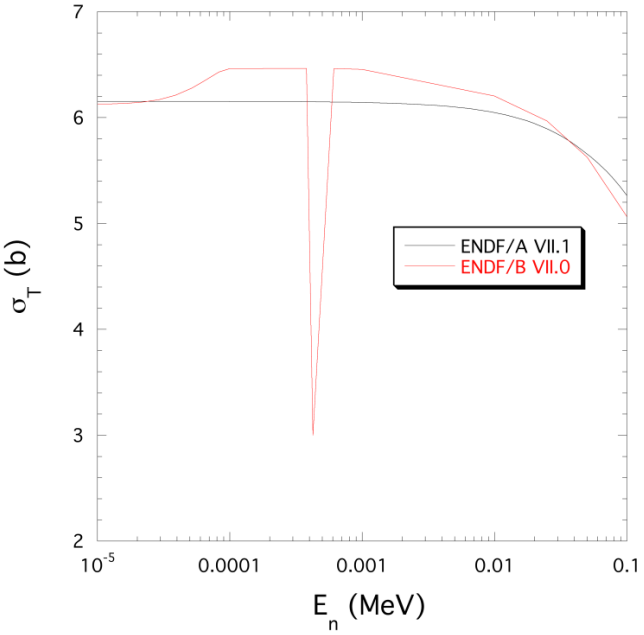
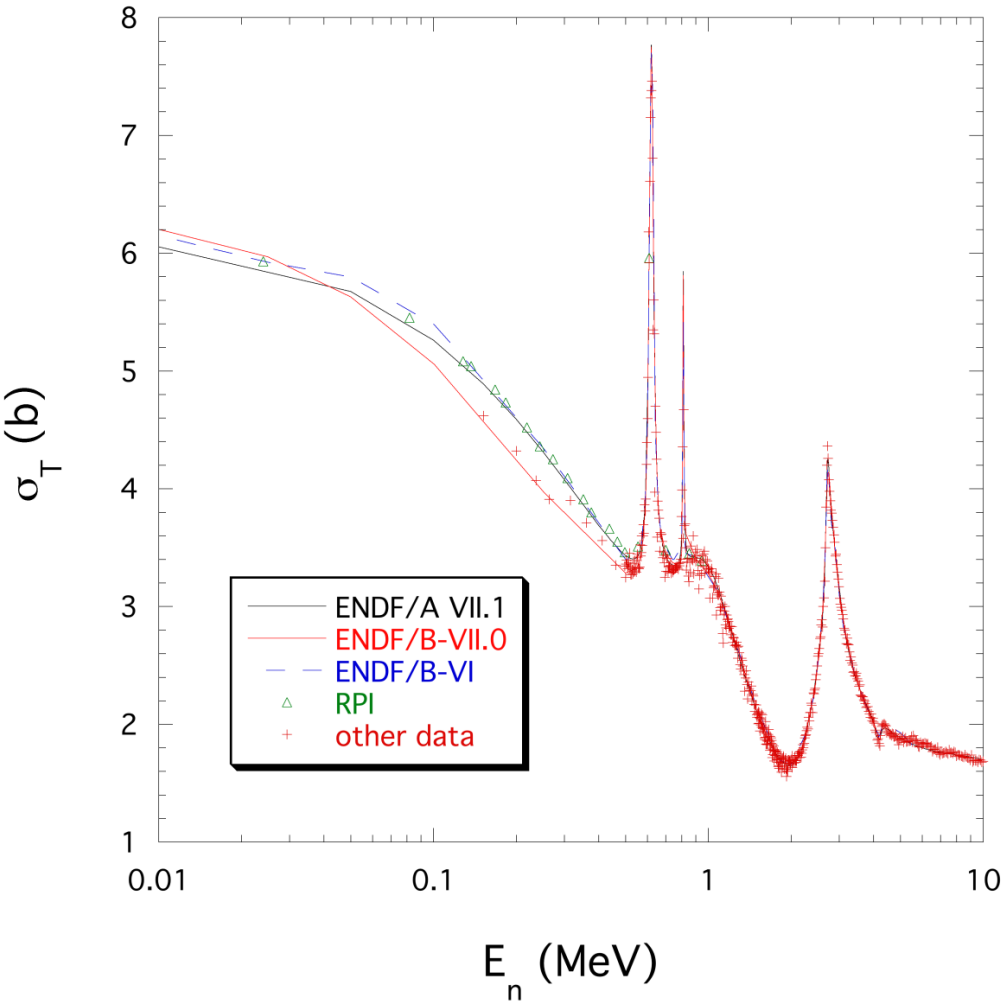
Nuclear Data – Evaluations – ^{9}Be



ENDF/A:

- "Glitch" in σ_{tot} removed
- Better fit to RPI data below 500 keV



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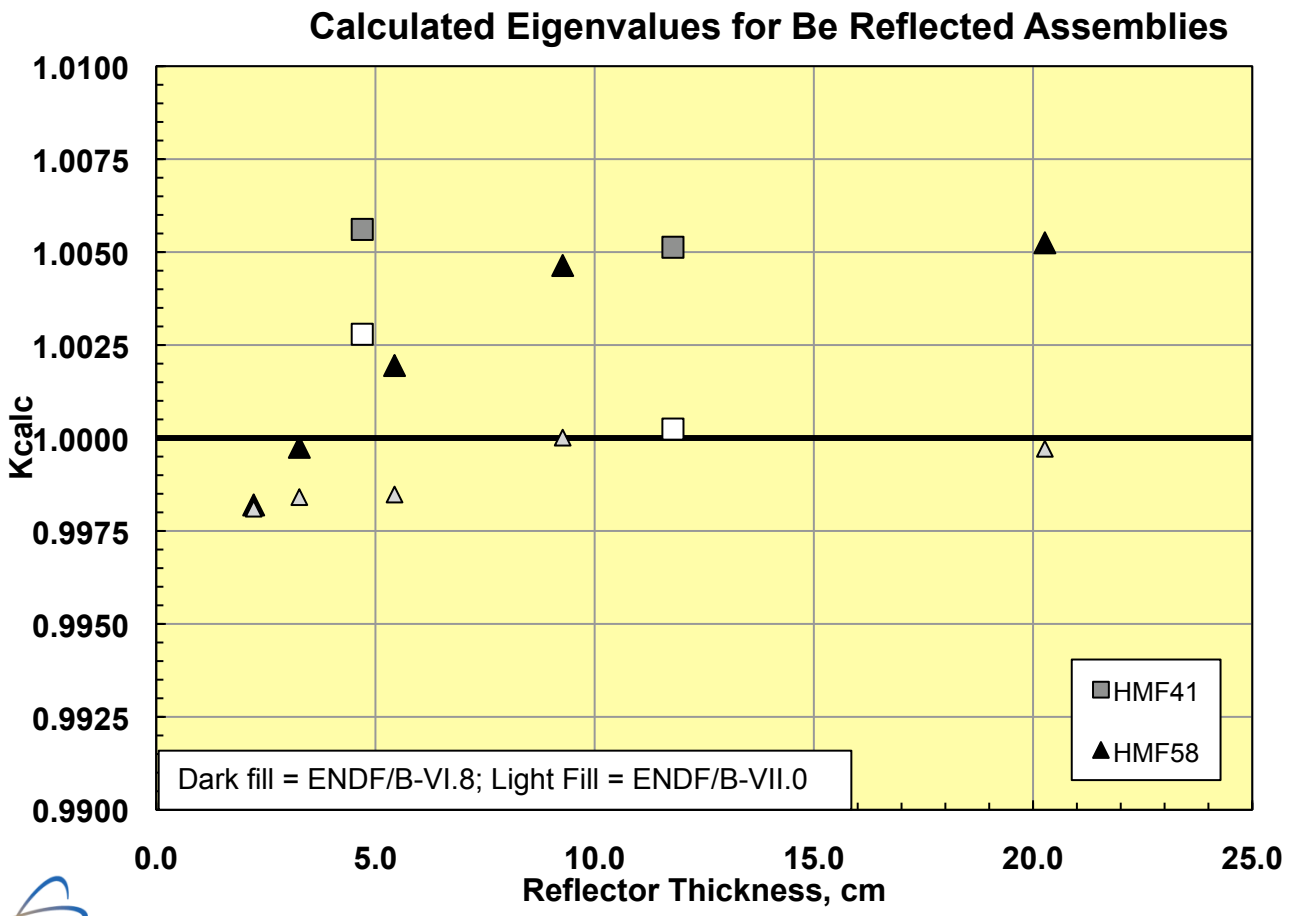
Nuclear Data – Evaluations – ^{9}Be



- LANL & LLNL experiments
- E68 k_{calc} biased high
- E70 k_{calc} is improved
- but …

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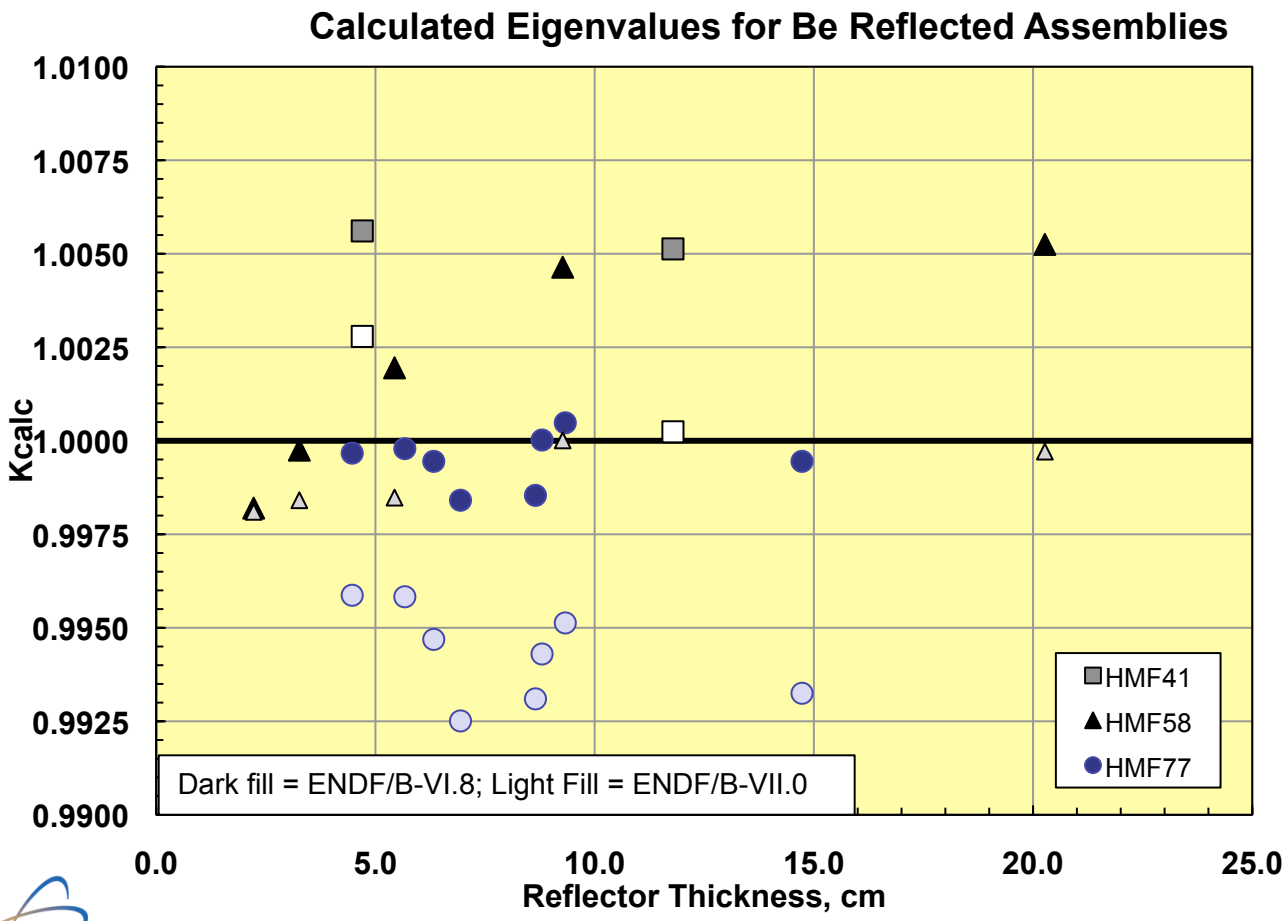
Nuclear Data – Evaluations – ^{9}Be



- LANL & LLNL experiments
- HMF58 & 77 are LLNL experiments that use the same components!

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Nuclear Data – Evaluations – ^{16}O

- Small changes in σ_{el} and σ_{tot} at energies below 7.5 MeV.
- Scale of $\sigma_{n\alpha}$ cross section increased about 35% below 9 MeV, putting it back about where it was before the previous change.
- All cross sections above 9 MeV are unchanged.
- Little change in already good k_{calc}; calculations of the "broomstick" transmission measurement are underway (but this is a low-resolution experiment).
- Covariances are given for the major cross sections, and for the first elastic scattering Legendre coefficient.

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Nuclear Data – Evaluations – ^{16}O

channel	a_c (fm)	l_{max}
n+^{16}O	4.3	4
α+^{13}C	5.4	5

Reaction	Energies (MeV)	# data points	Data types
$^{16}O(n,n)^{16}O$	$E_n = 0 – 7$	2718	σ_T, $\sigma(\theta)$, $P_n(\theta)$
$^{16}O(n,\alpha)^{13}C$	$E_n = 2.35 – 5$	850	σ_{int}, $\sigma(\theta)$, $A_n(\theta)$
$^{13}C(\alpha,n)^{16}O$	$E_\alpha = 0 – 5.4$	874	σ_{int}
$^{13}C(\alpha,\alpha)^{13}C$	$E_\alpha = 2 – 5.7$	1296	$\sigma(\theta)$
total		5738	8

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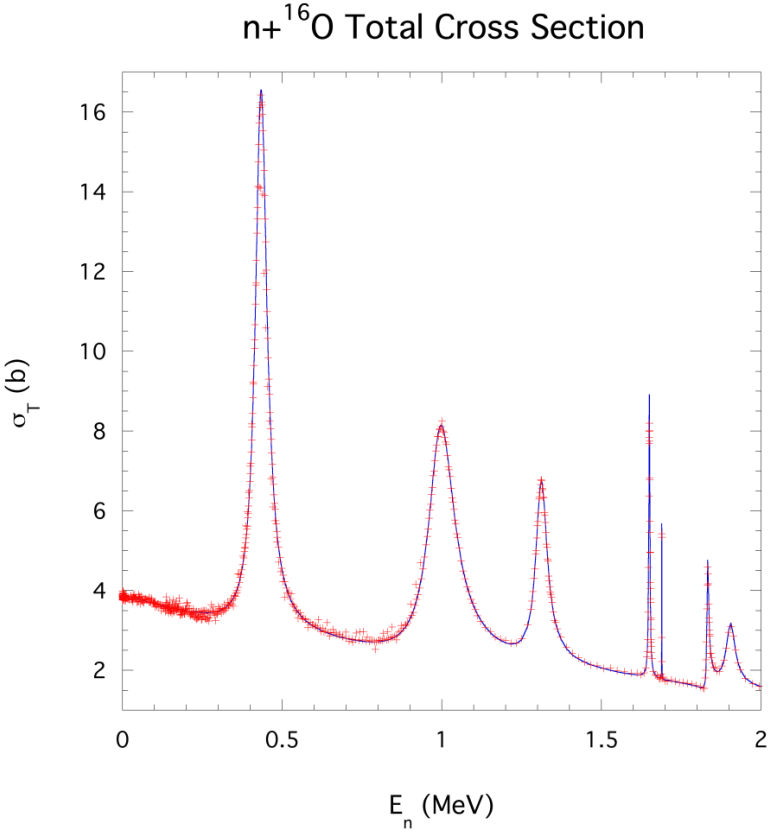
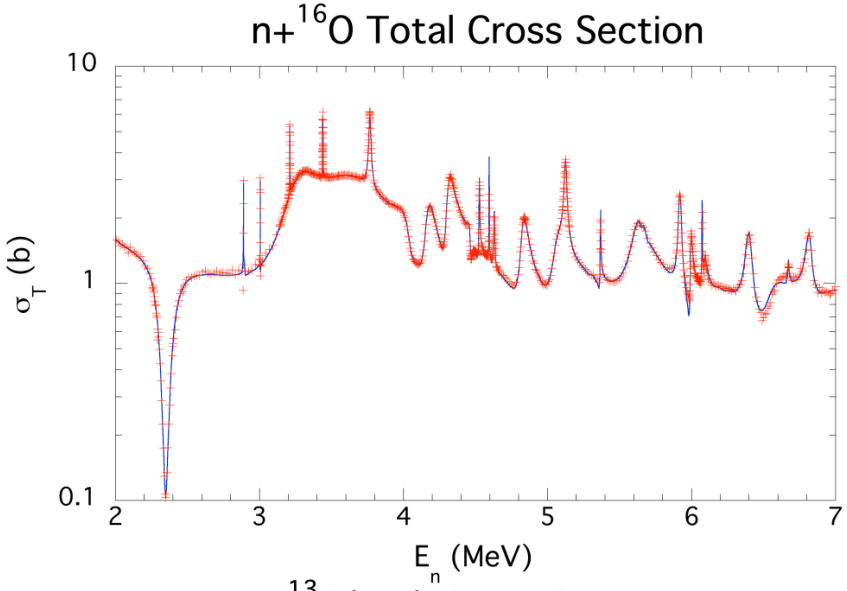
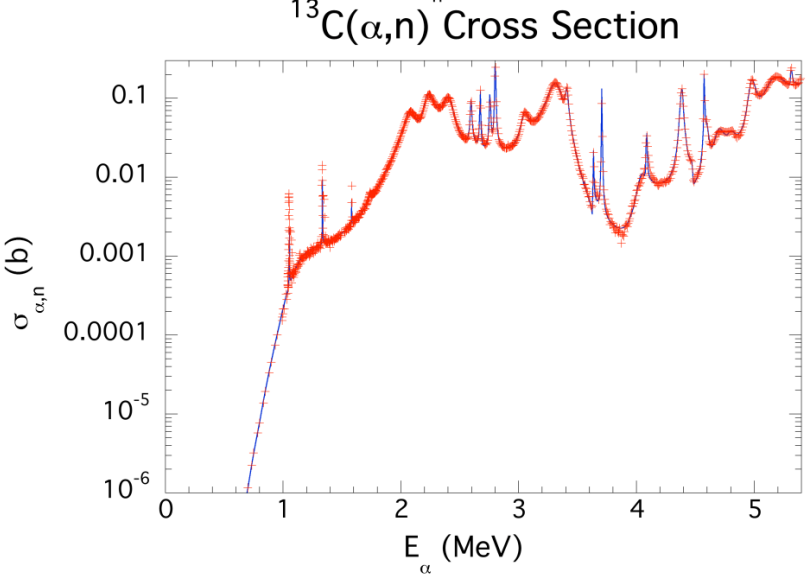
Nuclear Data – Evaluations – ^{16}O







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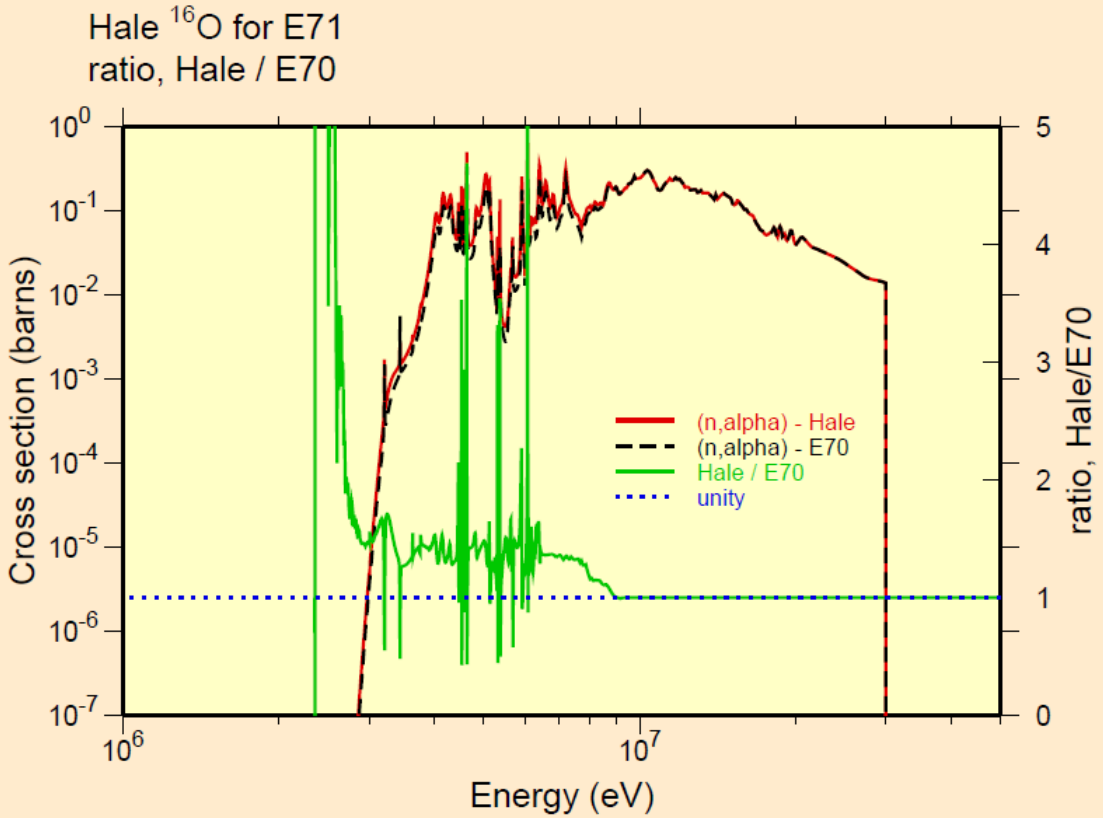
Nuclear Data – Evaluations – ^{16}O



- Most significant revision in this re-evaluation is to the (n,α) cross section from threshold to ~9 MeV.

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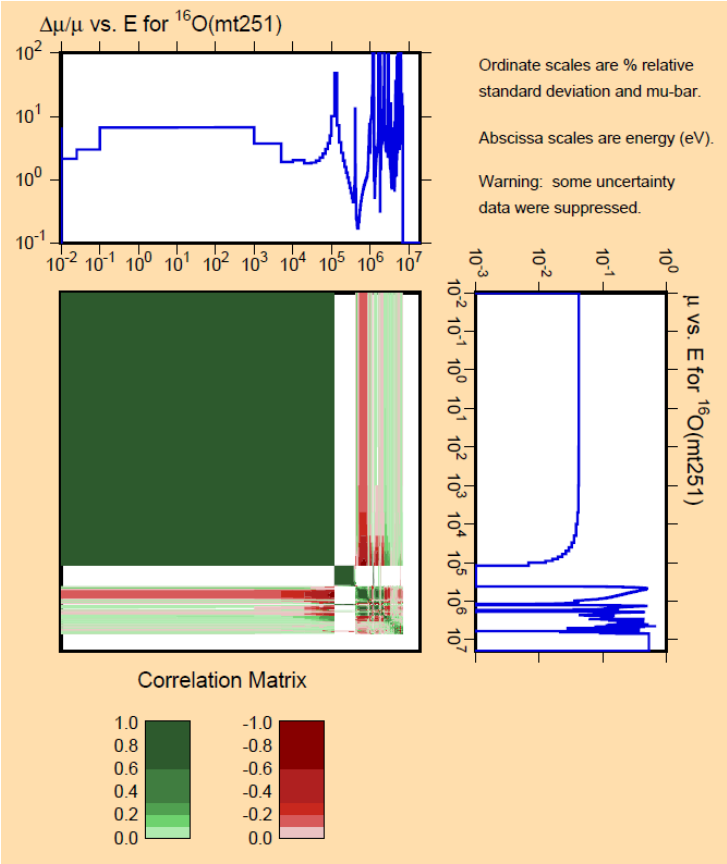
Nuclear Data – Evaluations – ^{16}O



- NJOY Processed MF34 Data.

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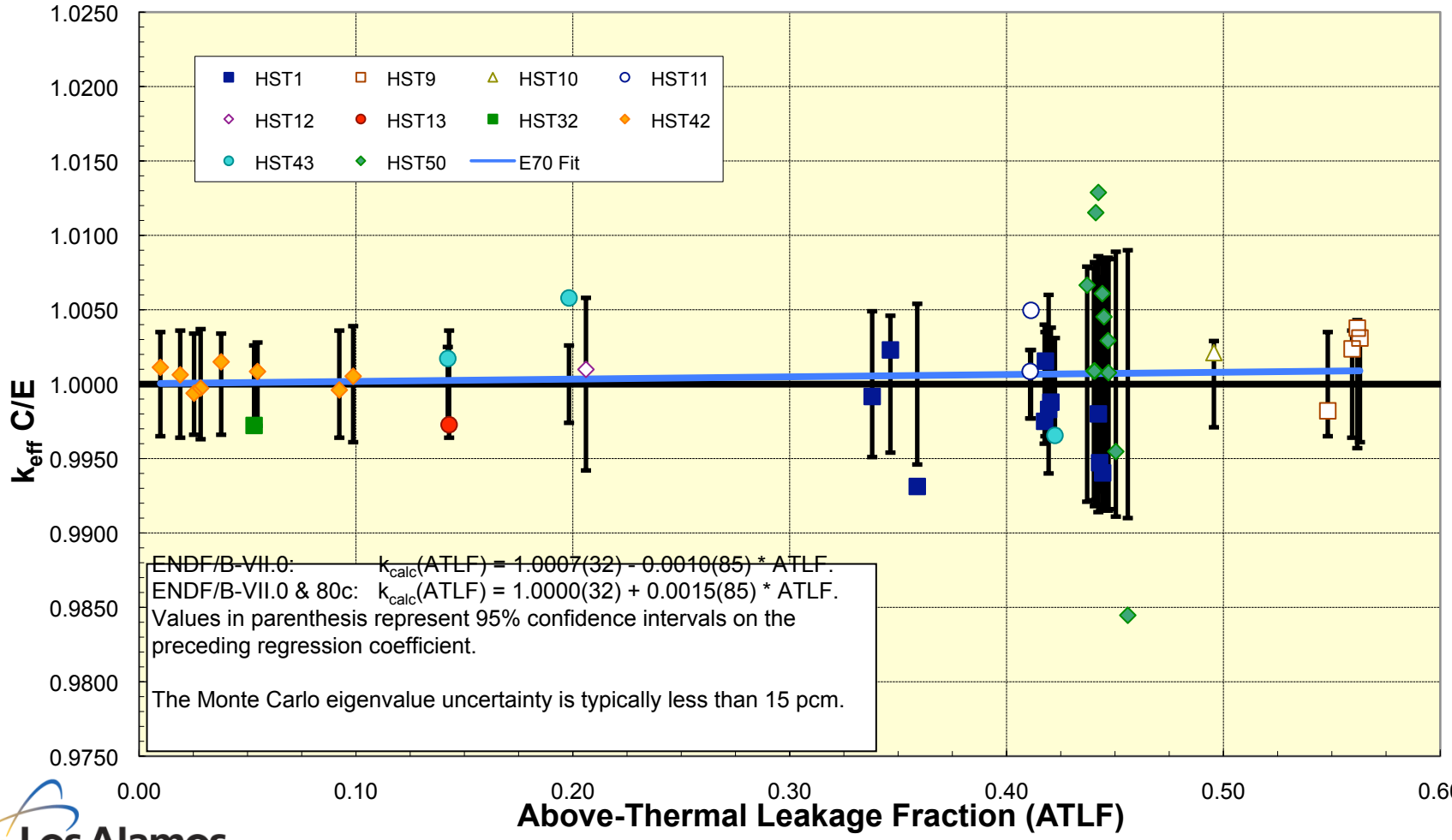
Nuclear Data – Evaluations – ^{16}O



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Nuclear Data – Evaluations – Vanadium

- $^{50,51}V$
  - Elemental ENDF/B-VII.0 evaluation will be replaced by isotopic evaluations; adopt JENDL-4 for ^{50}V; new evaluation for ^{51}V.
- For ^{51}V:
  - Total Cross Section
    - 100 keV - 5 MeV adopt JENDL-4; above 5 MeV, optical model calculations using a modified Koning-Delaroche potential.
  - Reaction Cross Sections
    - all cross sections above 100 keV were evaluated consistently with the Hauser-Feshbach code CoH.
  - Scattering Angular Distributions
    - Retain elemental ENDF/B-VII.0 elastic scattering data
    - Use COH calculated results for inelastic levels.

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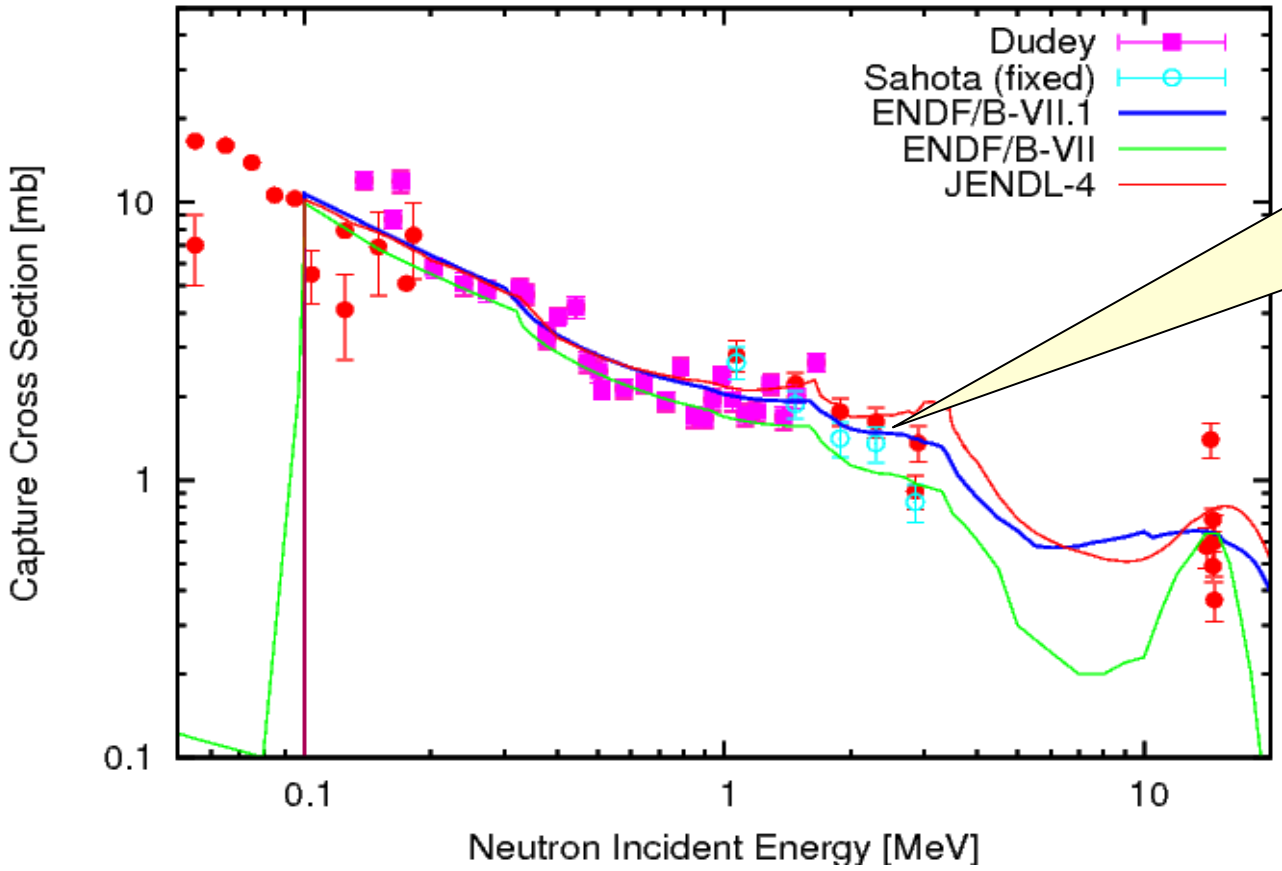
Nuclear Data – Evaluations – Vanadium (^{51}V)



Exp. data of Sahota et al. corrected by using updated reference cross section

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Data Testing: Ti and V Benchmarks

- Data Testing with ICSBEP Ti and V bearing benchmarks
  - Ti
    - HMF34 (case 1): interleaved HEU/Ti/Al.
    - HMF79: 5 cases with increasing axial reflector thickness.
    - HMM1: interleaved HEU/Ti/polyethylene plus a radial poly reflector.
    - HMM15: interleaved HEU/Ti/polyethylene plus a radial poly reflector.
  - V
    - HMF25: 5 cases with increasing axial reflector thickness.
    - HMF40: interleaved HEU/V.
    - HMM16: axial V with interleaved HEU/polyethylene.

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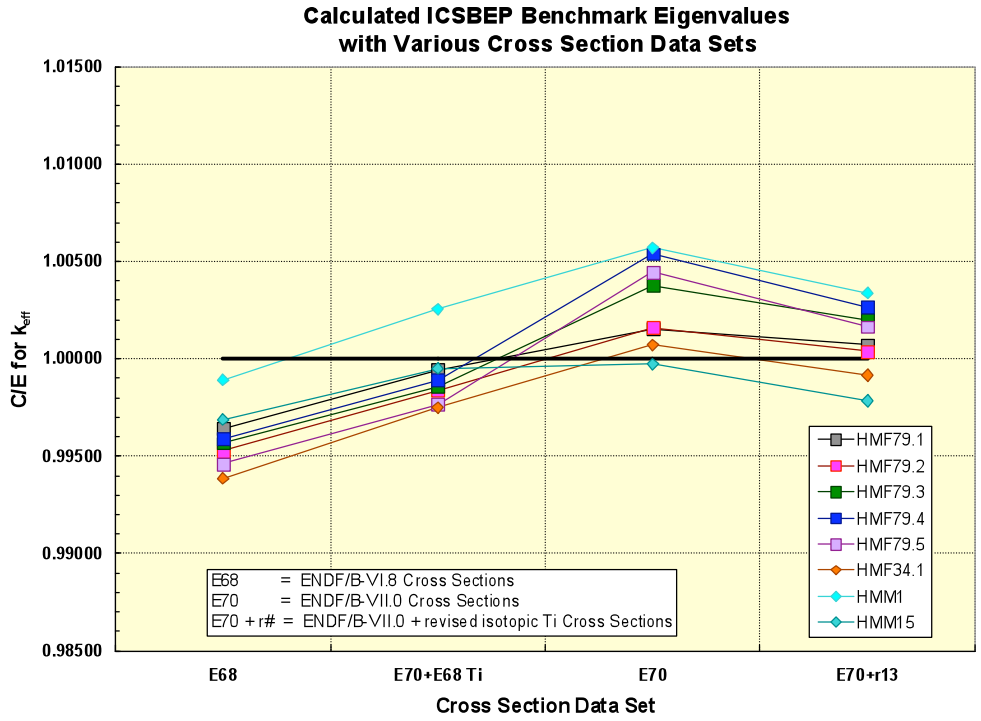
Data Testing: Ti Benchmarks



- ENDF/B-VII.0 based eigenvalues are less accurate than those obtained with ENDF/B-VI.8.
- Revised LANL Ti isotopic data sets eliminate much of this deficiency.
  - Average calculated eigenvalues are still biased high.

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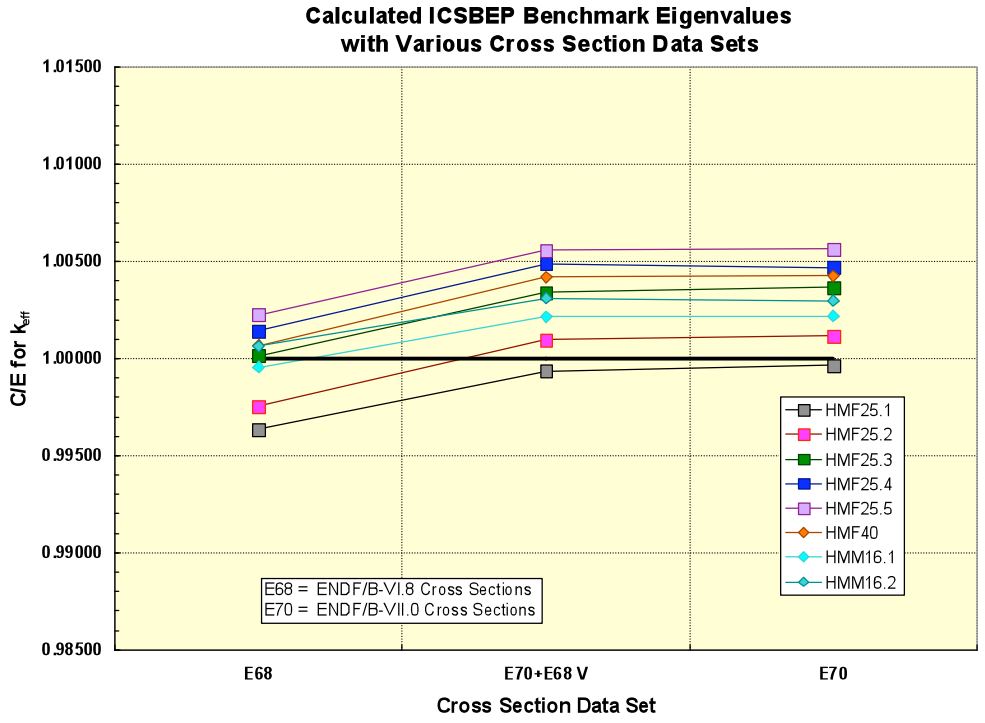
Data Testing: V Benchmarks



- Average calculated eigenvalue is too high.
- HMF25.x exhibits increasing calculated eigenvalue trend with increasing axial reflector thickness.

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Data Testing: Ti and V Benchmarks

- Conclusions
  - Eigenvalues for Ti bearing benchmarks are calculated more accurately with the latest LANL generated isotopic Ti data files.
    - The increasing calculated eigenvalue trend introduced with the current ENDF/B-VII.0 isotopic Ti data sets has been significantly reduced.
  - ENDF/B-VII.0 V is a carryover from ENDF/B-VI, evaluated by ANL in the late 1980's, with minor revisions by BNL. These integral data testing results suggest there may be deficiencies in either the elastic scattering angular distributions and the secondary energy distributions.

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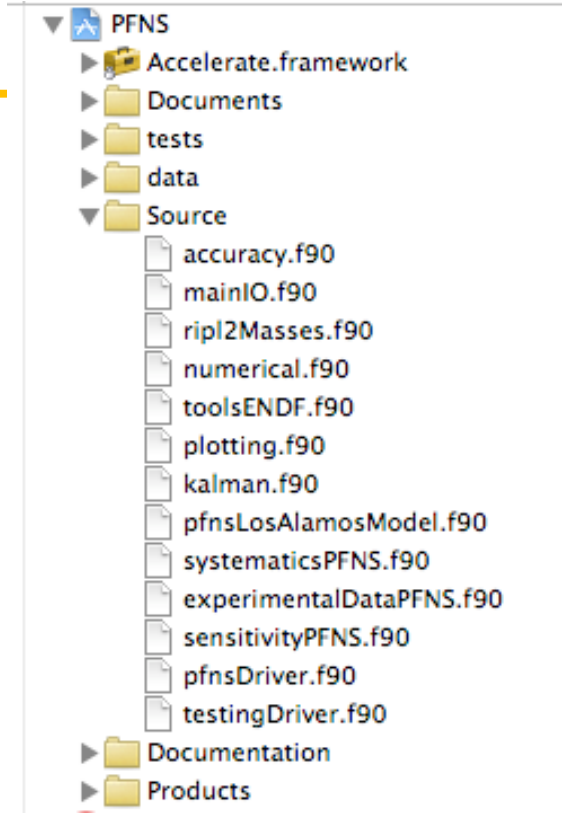
PFNS Evaluation Package

- Complete code package to analyze, compute and evaluate prompt fission neutron spectrum and multiplicity
  - Implementation of the Madland-Nix model
  - Model input parameter systematics included
  - Complete module to analyze various experimental data sets
  - Search for optimal model parameters
  - Uncertainty Quantification of spectrum and multiplicity
  - ENDF formatting for easy incorporation in evaluated libraries
- Version 1.0 released (internally)
- AFCI-NEUP collaboration with A.Prinja, M.Rising, UNM
- First application to suite of plutonium isotopes
- Ongoing:
  large suite of actinides studied to replace values in ENDF/B-VII.0



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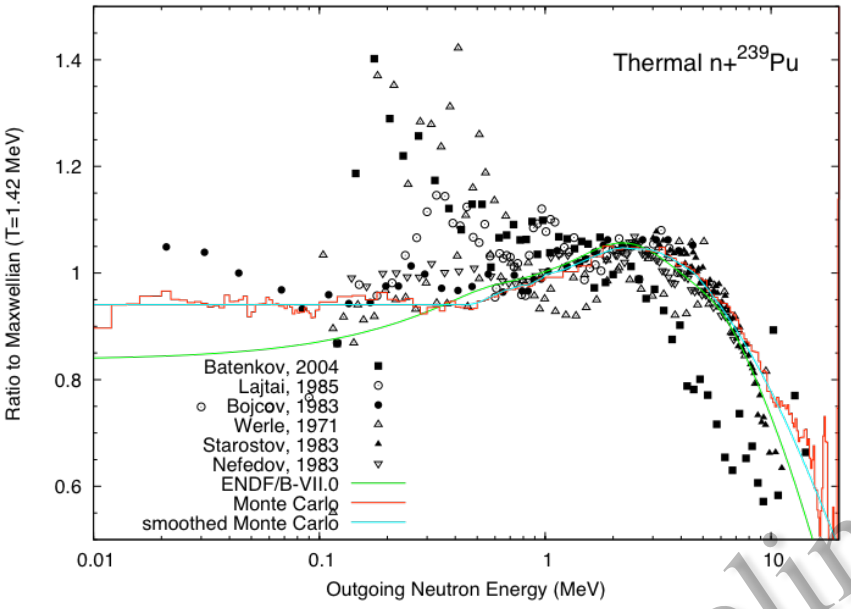
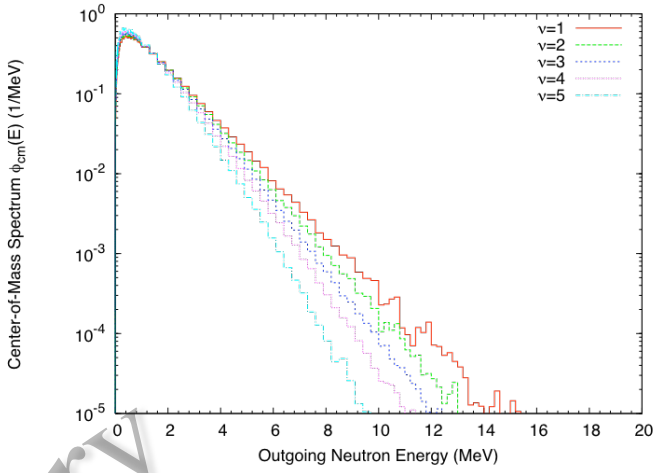
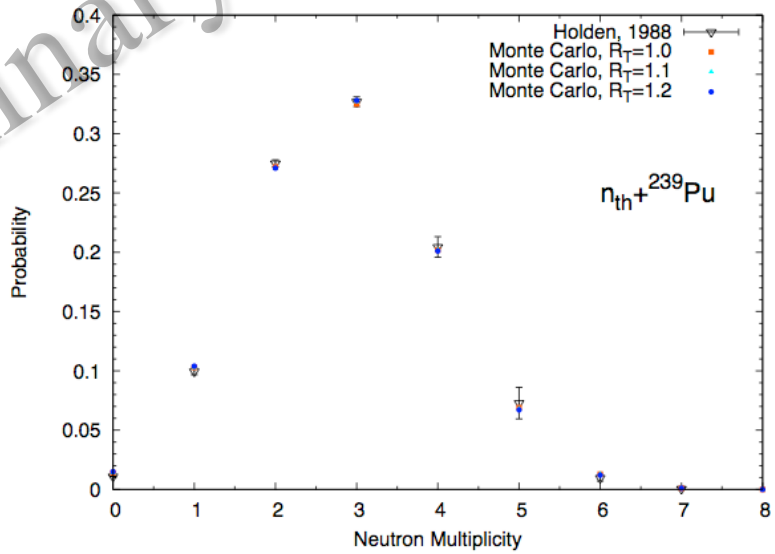
PFNS Evaluation Package







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Nuclear Data – Evaluations – ^{237}Np

- Revised (n,2n) and (n,3n) cross sections
  - Include ^{236,236m}Np production based upon Maslov evaluation.
  - MT=1 & MT=3 adjusted to remain consistent with these revisions.

- C/E for ^{237}Np(n,2n)/^{235}U(n,f) in Godiva, Flattop-25 and Big-10 remain high, but are closer to unity.